

## IV.B Hydrogen from Coal

### IV.B.1 The Integration of a Structural Water-Gas-Shift Catalyst with a Vanadium Alloy Hydrogen Transport Device

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*For this project, the Western Research Institute will partner with the Department of Chemical and Petroleum Engineering at the University of Wyoming.*

### Objectives

Produce a scalable device that can perform both the water-gas-shift (WGS) and hydrogen separation functions for a stream of synthesis gas derived from gasification of coal. This is to be accomplished via the following activities:

- Develop an improved monolithic WGS catalyst that provides efficient conversion of carbon monoxide and structural support for a stacked assembly of membranes.
- Demonstrate an improved vanadium alloy hydrogen transport membrane suitable for the chemical and physical environment of the coal-derived synthesis gas stream.
- Demonstrate devices that are scalable for commercial operation and designed for economic mass production via an integrated stacked catalyst and membrane assembly.

### Technical Barriers

This project addresses the following technical barriers from the Hydrogen Production section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

- L. Durability
- O. Selectivity
- Q. Flux
- S. Cost

The project also addresses one or more of the barriers described in Section 5.1.5.1., Technical Barriers – Central Production Pathway in the Hydrogen from Coal – Research, Development, and Demonstration Plan of the DOE Office of Fossil Energy.

## Technical Targets

This project consists of three steps for the improvement of hydrogen production. The first is an improved monolithic WGS catalyst that provides efficient conversion of carbon monoxide as well as a structural support for a stacked assembly of membranes. The second is an improved vanadium alloy hydrogen transport membrane that is stable in the chemical and physical environment of a coal-derived synthesis gas stream. The third is a scalable, integrated catalyst and membrane assembly that is designed for economic mass production.

Insights gained from these studies—in particular, the scalable, integrated catalyst and membrane assembly designed for mass production—will help meet DOE's 2010 and 2015 hydrogen production and separation targets, particularly with respect to membrane/module cost, durability, operating pressure, hydrogen recovery, and hydrogen quality. These targets are shown in Tables 1 and 2.

**Table 1.** Technical Targets: Ion Transfer Membranes for Hydrogen Separation and Purification<sup>a</sup>

Performance Criteria	Units	2003 Status	2005 Target	2010 Target	2015 Target
Flux Rate	scfh/ft <sup>2</sup>	60	100	200	300 <sup>b</sup>
Cost	\$/ft <sup>2</sup>	2,000	1,500	1,000	<\$500
Durability	Hours	<8,760	8,760	26,280	>43,800
ΔP Operating Capability	psi	100	200	400	400-1000
Hydrogen Recovery	% of total gas	60	>70	>80	>90
Hydrogen Purity	% of total (dry) gas	>99.9	>99.9	>99.95	99.99

<sup>a</sup> Targets are derived from Table 3.1.5. from the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan, March 2005.

<sup>b</sup> Flux upper limit for ion transport membranes.

**Table 2.** Technical Targets for the Water Gas Shift Reaction

Performance Criteria	Units	Current Status	2005 Target	2010 Target	2015 Target
Reactor Type	–	Multiple fixed beds		To be determined	
Catalyst Form	–	Pellets		To be determined	
Active Metal	–	Cu/Zn or Fe/Cr or Co/Mo		To be determined	
Temperature	°C	200-550	300-450	300-500	200-600
Pressure	psia	450-1150	450	750	>1,000
Approach to Equilibrium	°C	8-10	10	6	>4
Min Steam/CO Ration	Molar	2.6	3.0	2.5	<2
Sulfur Tolerance	–	Varies	Low	Moderate	High
Chloride Tolerance	–	Varies	Low	Moderate	High
Water Tolerance	–	Varies	Low	Moderate	High
Stability/Durability	Years	3-7	3	7	>10
Reactor Cost Reduction	%	–	–	>15%	>30%

<sup>a</sup> Targets are derived from Table 6 of the Hydrogen from Coal RD&D Plan, June 10, 2004.

## Approach

- Develop an improved vanadium alloy hydrogen transport membrane that can handle the chemical and physical environment of the coal-derived synthesis gas stream.
- Design and construct an integrated catalyst and membrane stack, where the assembly is scalable for economical commercial manufacture.
- Test the device for pressure integrity, hydrogen transport, compression strength, catalyst activity, and performance improvements over current technology.

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## Introduction

There exists a research need to develop a system that combines WGS technology with separation technology for coal-derived synthesis gas. The justification of such a system would be improved efficiency for the overall hydrogen production. By removing hydrogen from the synthesis gas stream, the WGS equilibrium would force more carbon monoxide to carbon dioxide and maximize the total hydrogen produced. Another benefit is the reduction in plant capital cost by the removal of one step in the process by integrating the WGS reactor with the membrane separation device.

## Approach

This project consists of three steps for the improvement of the hydrogen production system: 1) an improved monolithic WGS catalyst that provides efficient conversion of carbon monoxide and structural support for a stacked assembly of membranes; 2) an improved vanadium alloy hydrogen transport membrane suitable for the chemical and physical environment of the coal-derived synthesis gas stream; and 3) an integrated stacked catalyst and membrane assembly scalable for commercial devices and designed for economic mass production. The structural WGS catalyst will have a formulation that will eliminate the friable nature of current iron oxide based pellets. The shape of the catalyst will be important in the structure. Standard ceramic processing techniques will be used to formulate, mix, extrude and sinter porous corrugated

sheets of catalyst. Testing of the ceramic for catalytic activity and compression strength will be conducted.

The next step in this approach is the development of an improved vanadium alloy hydrogen transport membrane that can handle the chemical and physical environment of the coal-derived synthesis gas stream. A series of ternary vanadium alloys will be selected from previous research on vanadium alloys as hydrogen transport materials. They will be enhanced for improved brazing performance, after which they will be fabricated into foils and tested for hydrogen sulfide, steam and chlorine stability; hydrogen flux; braze strength; and hydrogen embrittlement resistance versus temperature and hydrogen concentration.

In the final step, an integrated catalyst and membrane stack will be designed and constructed, where the assembly is scalable for economical commercial manufacture. The device will be tested for pressure integrity, hydrogen transport, compression strength, catalyst activity, and performance improvements over current technology. The tests will be conducted in a syngas stream from a fluidized bed coal gasifier located at the Western Research Institute.

## Accomplishments

This project is newly initiated and no there are no accomplishments to report to date.